

Long-time unbreaking correlations in the large number of degrees of freedom Hamiltonian system

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Abstract

A behaviour of molecular cluster with Lennard-Jones potential of interactions as Hamiltonian system is studied by computer simulation (molecular dynamics method). It is shown that complex periodic oscillations of the cluster as a whole are possible. This is in accordance with KAM theorem.

1 Introduction

We study the behaviour of the dynamical system with Lennard - Jones interaction by computer simulation. The main physical motivation is concerned with long - time dynamical evolution in nonlinear Hamiltonian systems perturbed by random fluctuations caused by rounding-off errors.

The goal of works [1-4] was the investigation of a dynamical foundations of classical statistical mechanics. It were considered :

- a chain of N nonlinearly coupled particles whose Hamiltonian is given by [3] (Fermi - Pasta - Ulam β - model)

$$H = \sum_{i=1}^N \left(\frac{1}{2} \dot{\phi}_i^2 + \frac{1}{2} (\phi_i - \phi_{i+1}) + \frac{1}{4} \beta (\phi_i - \phi_{i+1})^4 \right) \quad (1)$$

where ϕ_i are the displacement with respect to stable positions.

- a chain of N nonlinearly coupled particles with Hamiltonian [3]

$$H = \sum_{i=1}^N \left(\frac{1}{2} \dot{\phi}_i^2 + \frac{1}{2} (\phi_i - \phi_{i+1}) + \frac{\alpha}{3} (\phi_i - \phi_{i+1})^3 \right) \quad (2)$$

- the system of N particles arranged on a square lattice with nonlinear interaction through a Lennard - Jones potential [1]

$$V(r) = 4\epsilon \left(A_1 \left(\frac{\sigma}{r} \right)^{12} - A_2 \left(\frac{\sigma}{r} \right)^6 \right) \quad (3)$$

ϵ is a depth of the potential well;
 $\sigma = r_0 2^{-1/6}$, where $V(r_0) = 0$, in [1-2] were taken $A_1 = 1, A_2 = 1$.
Boundary conditions have been chosen periodic in normal mode coordinates [3]

$$\phi_i = \phi_{i+N},$$

or square lattice was surrounded by a border of fixed particles [1-2].

In all cited works it have been proposed that particles oscillate about their stable positions. The main results there obtained may be summarized as follows:

- at low energy there exist ordered motions, normal modes appear to be uncoupled [2];
- correspondingly to a certain value of the average - time kinetic energy per particle relaxation toward the equilibrium is strongly slowed down [4];
- a time of relaxation $\tau_r(\epsilon)$ (ϵ is a full energy per particle in normal modes terms) is compatible with Nekhoroshev - like low [4] with model dependent parameter δ

$$\tau_r = \tau_0 \exp\left(\left(\frac{\epsilon_0}{\epsilon}\right)^\delta\right) \quad (4)$$

At high energy the transition between ordered - disordered (weakly - strongly chaotic dynamics) occurs but there are no exist thresholds between two dynamical regimes. In all cited papers the choice of an indicator of system's state was found to be insufficient. The use of relaxation time $\tau_r(\epsilon)$ is initial conditions dependent [4], spectral entropy $\eta(t)$ is different from zero when $t \rightarrow \infty$ [3-4], Laypounov characteristic exponent $\lambda(\epsilon)$ is initial conditions independent but gives model - dependent transition and poor convergence when number of particles N is large.

The main physical conclusion is the following: " there is a nonvanishing measure of initial conditions in phase space that can originate long living metastable states even in the thermodynamical limit " [4].

It has been studied Hamiltonian dynamics subjected to rounding - off errors fluctuations. The tests concerned the Hamiltonian dynamics were the following: negligibly small value of $\Delta\epsilon/\epsilon \simeq 10^{-5} - 10^{-6}$ and time reversible dynamics for $t \rightarrow -t$ [4].

Based on cited results it may be concluded that:

- with the proviso that particles oscillate close to positions where their potential energy has a minimum, provided that number of the positions equal to number of particles, when full energy $\epsilon > \epsilon_c$ (ϵ_c is model and initial conditions dependent) a number of oscillations with continuous random spectrum may increase on account of decrease in oscillations with discrete spectrum;
- apparently in general way a characteristic time $\tau_r^{(1)}(\epsilon)$ for breaking of discrete spectrum is not existent;
- a finite characteristic time $\tau_r^{(2)}(\epsilon)$ within which one would to determine a

random nature of oscillations in system is not existent;
- there is a fundamental problem of long - time following of dynamics in computer simulations because of rounding - off errors. This are nearly tangent to problem of modelling of dynamical evolution.

The starting positions of the work based on assumption that weak changes of oscillations modes in dynamical system with large number of degrees of freedom may give rise to complex behavior of whole system when to abandon any restriction in motions and in particular one could to observe the dynamics without any changes in oscillations modes during long - time computer simulations with unbreaking correlations of the motions in a whole system despite of rounding - off errors.

2 Model description

Computer simulation runs have been performed for N particles Lennard -Jones system without any boundary or the like conditions. The equations of motion have been computed with undimensional time - step $\Delta t = 0.05 - 0.13$, where real time - step

$$\Delta t_{real} = \Delta t \left(\frac{m\sigma^2}{48\epsilon} \right)^{1/2} \quad (5)$$

The undimensional average - time kinetic energy per particle is defined as follow

$$\langle \epsilon_{kin} \rangle = \frac{1}{N} \sum_{i=1}^N \langle (v_{xi}^2 + v_{yi}^2) \rangle \quad (6)$$

Computer simulations were carried out without any cut off range of r .

Initial conditions are of particular significance in present work. The starting points of particles are setting up as follows

$$x_i = \alpha A j \sin \left(\frac{2\pi i}{N_i} \right), y_i = A j \cos \left(\frac{2\pi i}{N_i} \right) \quad (7)$$

$A = 6.752/4.53$, $N_i = 22$ when $j = 4, i = 1 \dots 22$, and $N_i = 32$ when $j = 5, i = 1 \dots 32$, and $N_i = 44$ when $j = 6, i = 1 \dots 44$, $\alpha = 1.013$, $A_1 = 4.870$, $A_2 = 1$.

At the first stage of formation of the cluster next scaling way was used. After time $t = 200k\Delta t, k = 1 \dots 5$, over the particles velocities were set $v_{xi} = 0, v_{yi} = 0$ for $i = 1 \dots N$. After some time t_1 the scaling of velocities was abandoned and the cluster became as isolated but subjected to rounding - off errors. So the dynamical system is Hamiltonian or near Hamiltonian as fluctuations of full energy $\Delta\epsilon/\epsilon$ were of the order of $10^{-4} - 10^{-5}$ and average - time $\langle \Delta\epsilon \rangle$ was equal to zero.

3 Results description

The graphical displays of the cluster during program runs is depicted in Fig.1. The cluster oscillates as whole with period $t^* \simeq 2000$ and is unbreaking by rounding - off errors (in this case the time of the unbreaking correlations of motion of cluster as a whole was $t_r = 5 \cdot 10^4$, time step $\Delta t = 0.13$). The dependence of time of an unbreaking correlations vs its full energy per particle is reported in Fig.2 ($t_1 = 1100$ in this case). In Fig.3 is shown the value of average kinetic energy per particle. It is displayed time - average kinetic energy $\langle \epsilon_{kin} \rangle$ though all particles of the cluster has a complex periodic oscillations about some state (Fig.4).

The cluster doesn't lose this complex periodic oscillation when time - step of integration was 2 times increased and doesn't lose its symmetry when program runs ($t_r = 10^5$, time - step $\Delta t = 0.13$) in the case when full energy per particle is about 0.01 (in undimensional units).

The number of particles with similar symmetrical behavior is no less then two - fold.

4 Discussion

In accordance with KAM theorem such cluster with complex periodic oscillations is possible.

What is to bring out the existence in computer simulation such cluster?

- the cluster has sensitivity to initial conditions and to parameters A_1, A_2 of potential of interaction. All of this are characteristic for chaotic system.
- the cluster brings out the unbreaking collective correlations. The average - time kinetic energy equal to 1-3 K (parameters ϵ, σ were taken for argon). This is the interval of an energy where convergence of normal modes in questionable in accordance with [1-2].
- collective correlations of the motion increase the stability of the cluster as a whole despite of rounding - off errors.

Is the cluster artificial or has its physical reality ? This is out of the purpose of the present work. The dynamics of the cluster is near Hamiltonian with $\langle \epsilon \rangle \simeq const$.

We would like to underline that symmetry in initial position of the particles brings complex periodic oscillations in this case. For the cluster with parameters $A = 6.752/4.53, N_i = 20$ when $j = 4, i = 1 \dots 20, N_i = 30$ when $j = 5, i = 1 \dots 30, N_i = 40$ when $j = 6, i = 1 \dots 40, \alpha = 1.000, A_1 = 4.870, A_2 = 1$. one could to observe spontaneous turning of symmetry axis induced by rounding - off errors. Spontaneous breaking or turning of symmetry of any kind in Hamiltonian dynamics is impossible.

Some words about description parameters of the cluster where one could observe contraction - extention of the cluster as a whole. When time - space scale

is large then one needs only 4 parameters to describe contraction - extention of the cluster as a whole. For molecular space and time scale one needs much more number of degrees of desription's parameters (but less then $4N$).

There is main question from the work. We would like to formulate this question as follow: What number of degrees of freedom, full energy and potential of interaction did provide time of an unbreaking correlations in a cluster subjected to rounding - off errors for an infinity or this time is always finite ?

References

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